

Procedure for Exporting Main (Single Structure) ChemFinder (CFW) file to DSSTox SDF using ChemOffice 2000 ChemFinder (ver. 7.0): (14Jun03)

Order fields as in FieldDefFile and as they should be ordered in SDF for import into other applications before exporting to SDF.

Option 1: If all fields have final correct labels, redraw boxes in form view of ChemFinder

1. Launch **ChemFinder**.
2. Select **Open** from the file menu.
3. Select the Main ChemFinder File
4. Print screen showing all fields; also print listing of FieldDefFile.
5. Select arrow button on left panel. Select all boxes and delete.
6. Redraw each field box in the order in which it appears in the FieldDefFile, label field according to contents, and fill in data by right clicking on white box and choosing appropriate field name.
7. If any field in record 1 is blank, enter the word 'blank' in field as placeholder in first record of SDF (ensures proper order of fields on import into CRD). Placeholder word can be deleted by user after SDF is imported into CRD for use.
8. Save ChemFinder file to new name.
9. Select **Export>>SDFFile** from **File** Menu.
10. **Save As** the standard name with the .sdf extension.

Option 2: If some fields need to be deleted, rearranged, or do not have final correct labels, modifications to SDF can be made using Excel.

1. Perform steps 8 and 9 above to create SDF from Main file in original form.
2. Launch **Excel**.
3. Select **Open** from the file menu.
4. Select **New** from the **File** menu (this step insures that the personal.xls file will not be edited).
5. Select **Add-in...** from the **Tools** Menu.
6. Check the box associated with ChemDraw for Excel (ChemFinder Version 7.0 2002 or later) or ChemFinder for Excel (ChemFinder Version 6.0 2001 or earlier).
7. Select **OK** (a new toolbar and menu will be displayed titled ChemDraw or ChemFinder respectively).
8. Select **Convert/Update Worksheet** from the **ChemDraw/ChemFinder** menu.
9. Select **Import Table** from the **ChemDraw/ChemFinder** menu.
10. Select the SD file to be modified.
11. Within Excel, can edit field names and field contents
12. To rearrange order of fields, be sure to insert blank column in desired location before cutting or copying field one wishes to move. Then delete superfluous field.
11. When all changes are made, select **Export Table** from the **ChemDraw/ChemFinder** menu.
12. Save as the standard file name for SDF.
13. **Yes** write over the existing file of the same name.

14. Copy or move SDF to empty folder and reimport into ChemFinder to check ordering and contents of fields.